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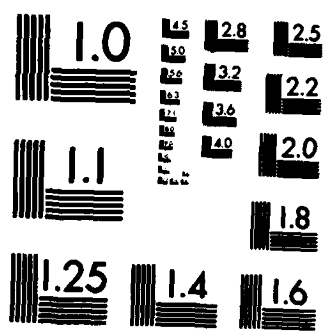
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

In this report we present a study of the optical and electrical properties of hydrogenated silicon-germanium alloys prepared by co-sputtering. The optical absorption coefficient α was evaluated both from optical transmission and from photoconductivity measurements. The data derived using the two methods are in good agreement. The values of α as a function of photon energy exhibit a shift to lower energies with increasing germanium content, indicating a decreasing band gap. For all the concentrations, the absorption coefficient drops rapidly

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with decreasing energy, indicating a fairly good structural order and low trap density.

The optical gap increases more or less linearly from 1.1 eV for 5 at.% Si to 1.7 eV for 70 at.% Si. The product $\eta\mu\tau$ (η-quantum efficiency, μ-mobility, and τ-recombination time) was derived from the saturation values of the photoconductivity. It decreases from $2x10^{-6}$ cm^2/V to a minimum of $2x10^{-9}$ cm^2/V as the silicon content decreases from 70% to 40% and then a slight rise as we near the germanium end. The variation of the optical gap with silicon concentration and the photoconductance response for our RF-sputtered films are similar to those reported by others for materials prepared by glow discharge. Thus it seems that the electrical and optical quality of our films is not inferior to glow-discharge ones.

The hydrogen content of the films was determined by nuclear resonant reaction with N^{15} ions. The total hydrogen content of the samples varied between 17 at.% for the germanium-rich end to 27 at.% for the silicon-rich end. From infrared absorption measurements we find that hydrogen bonds preferentially to Si over Ge by a factor of 10 - 15.

OPTICAL PROPERTIES OF COMPOSITE MATERIALS

Final Report

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September 15, 1984

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Statement of the Problem

The pioneering work of Spear and Le Comber[1] on hydrogenated amorphous silicon (a-SiHx) and of Carlson and Wronski[2] on a-SiH_x solar cells, set in motion a considerable effort to develope efficient and cheap a-SiH_x solar cells for large-scale electric power generation. For solar cell application, the material must have a sufficiently low density of gap states to keep electron-hole recombination at tolerable level. The optical gap E_g should be low enough to utilize the solar spectrum but high enough to yield a reasonably high open-circuit voltage. The theoretically highest achievable efficiency for an ideal semiconductor[3,4] is with E_g=1.4 EV, while a-SiH_x has an E_g around 1.7 eV. With hydrogenated amorphous silicon-germanium alloys, on the other hand, the E_g values achievable are in the proper range. Thus it would seem that hydrogenated a-Si_xGe_{1-x} alloys are good candidates for solar-cell material. In this report we present a study of the compositional dependence of the optical, infra-red and electrical transport properties of the a-Si_xGe_{1-x}:H alloy system.

Summary of Results

Experimental

The a-Si_xGe_{1-x}:H films were sputtered reactively in a conventional parallel plate RF (13.56 MHz) sputtering system using a gas mixture of 12 mTorr Ar and 1.4 mTorr H_2 and an RF power of 300 W with a cathode self-bias voltage of -1200 V. In order to produce a compositional gradient in the plane of the substrate we used for target two 15 cm dia. half discs of Si and Ge, each made out of scintered 99.999% pure powders of the elements. The substrates, 7059 glass (for optical and transport measurements) and crystalline Si (for IR) were mounted on an electrically grounded steel plate facing the target, in a plane parallel and 5 cm above the target. The steel plate was electrically heated to maintain the substrate temperature at 230^oC.

The substrates were 1/2" wide, 6" long and were positioned above the targets with the long axis perpendicular to the dividing line between the two targets. The Si-Ge films were about 13 cm long and 3 mm wide. For electrical measurements, 50 Cr contacts were deposited upon the substrate at 0.1" intervals prior to the deposition of the Si-Ge film, thus dividing the film into 49 samples.

To evaluate the composition of the film as a function of position along the film we used the procedure developed by Hanak.[5] In this method the measured film thickness is compared to a profile calculated by a superposition of the deposition rates of the two targets. The

compositions were also checked by x-ray fluorescence and by Auger Electron Spectroscopy and the results were in good agreement with the computed ones.

The optical absorption coefficient as a function of photon energy was evaluated both from optical transmission measurements and from photoconductivity. The analysis of the optical data followed the procedure outlined by Cody et al.[6] The intensity dependence of the photoconductivity was neasured for each sample and the photoconductivity results corrected as discussed by Chahed et al.[7]

One of the important variables which influences the optical gap and the density of electronically active defects in the alloys is the concentration and bonding configuration of hydrogen. The total hydrogen content of the films was determined by nuclear resonant reaction with N^{15} ions. To determine the distribution of hydrogen between the Si and Ge sites we measured the IR absorption spectra between 400 and 2200 cm^{-1}. For quantitative analysis we used the hydrogen stretching vibration bands between 1800 and 2200 cm^{-1}.

Results

The a-Si_xGe_{1-x}:H films were 5000-10000 A thick and the silicon concentration varied along the length of the film from about 5 at.% Si to about 70 at.% Si. The total hydrogen content of the samples varied between 17 at.% for the germanium-rich end to 27 at.% for the silicon-rich end. From absorption measurements in the infrared we computed the at.% of hydrogen on the Si and Ge sites. We used gaussian line shapes FWHM 100 cm^{-1},centered at 1880 cm^{-1},

1975 cm^{-1}, 2005 cm^{-1} and 2100 cm^{-1} for the Ge-H, $Ge{=}H_2$, Si-H and $Si{=}H_2$ stretching modes respectively, and used the areas under the gaussians as adjustable parameters to obtain best fits to the IR spectra. In agreement with previous works[8,9] we find that H bonds preferentially to Si over Ge. We find an enhancement factor b of 10 - 15 except at the silicon-rich end where b decreases to about 5. We notice that this is also the region where the total hydrogen content of the film is the highest (27 at.%). This may indicate that higher overall hydrogen content enhaces the attachment of H to Ge sites.

The optical band gaps, E_g, were determined by fitting the measured optical absorption coefficient α by the Tauc relation $(\alpha E)^{1/2}$ = const.$(E-E_g)$ for photon energies $E>E_g$. The results show a more or less linear decrease of the gap with decreasing Si concentration from about 1.7 eV to about 1.1 eV. Our values of $E_g(x)$ are similar to those of van Roedern et al.[10] on glow-discharge prepared films but they are systematically higher then those reported by other workers for sputtered films.[11]

Electrical conductivity measurements were made in the plane of the films. The dark conductivity of the films increased from 10^{-5} to 10^{-4} $ohm^{-1}cm^{-1}$ as x decreased from 0.7 to .05. Photoconductivity was used to determine the product $\eta\mu\tau$ (η--quantum efficiency, μ--mobility and τ--recombination time) using strongly absorbed light, at 2 eV, and a photon flux of 10^{14} cm^{-2}. The dependence of $\eta\mu\tau$ on x is qualitatively similar to that observed by von Roedern el al.[10] for photoconductivity: first an abrupt

decrease with decreasing x reaching a minimum at x=0.4 followed by a slow increase, as x approaches zero.

The variation of the optical gap with silicon concentration and the photoconductance response for our RF-sputtered films are similar to those reported by von Roedern el al.[10] for samples prepared by glow discharge. Thus it seems that the electrical and optical quality of our films is not inferior to glow-discharge ones. This seems to be indicated[12] also by the steep decrease of the optical absorption coefficient with decreasing photon energy for all the concentrations studied. The ease of preparation, however, of a variety of compositions at one run with the co-sputtering technique, makes this technique more feasible for systematic studies of the influence of deposition parameters upon film characteristics.

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List of Participating Scientific Personnel

Dr. Zvi S. Weisz	Principal Investigator
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Dr. James A. Muir	Principal Investigator
Dr. Yehuda Goldstein	Senior Research Associate
Mr. Samuel Hernandez	Research Associate
Mr. Raul Perez Sandoz	Graduate Student, received M.S. 1983
Mr. Luis A. Perez Colon	Graduate Student, received M.S. 1983

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